REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	21 March 1996	Final Report 10/1/92 -- 3/31/96

4. TITLE AND SUBTITLE
Multilevel Techniques in Large Scale Computation

5. FUNDING NUMBERS
F49620-92-J-0439

6. AUTHOR(S)
Stephen F. McCormick

AFOSR-TR-96

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of Colorado at Boulder
Campus Box 526
Boulder, CO 80309-0526

G217

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Scott Schreck, Major, USAF
AFOSR/NM
110 Duncan Avenue, Suite B115
Bolling AFB, DC 20332-0001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT
unlimited

12b. DISTRIBUTION CODE

DISTRIBUTION STATEMENT A
Approved for public release;
Distribution Unlimited

13. ABSTRACT *(Maximum 200 words)*

This final report on AFOSR project "Multilevel Techniques in Large Scale Computation" (AFOSR #F49620-92-J-0439) is described according to the following topics, which include examples of how these applications have led to important basic advances: first-order system least squares (FOSLS); electromagnetics and seismology; meteorology; multiscale atmospheric data assimilation; molecular dynamics; robust three-dimensional solvers; and parallel adaptive refinement.

19960520 066

14. SUBJECT TERMS
multigrid, multilevel, adaptive, computing, fluid dynamics, finite elements, electromagnetics

15. NUMBER OF PAGES
6

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
unclassified	unclassified	unclassified	

This final report on AFOSR project "Multilevel Techniques in Large Scale Computation" (AFOSR number F49620-92-J-0439) is described according to the following topics, which include examples of how these applications have led to important basic advances:

- *First-Order System Least Squares (FOSLS)*

  This relatively new methodology is aimed at developing a well-posed functional minimization principle for a broad class of partial differential equations. The goal is to provide a general formulation that is elliptic in each variable so that standard discretization and multigrid solution method yield optimal results. The project established such functionals together with a theoretical foundation for this approach for diffusion-reaction equations, connection-dominated flow, Stokes or Navier-Stokes equations, linear elasticity, Helmholtz equations, and problems with discontinuous coefficients.

- *Electromagnetics and Seismology*

  New multilevel methods for modeling very general wave phenomena have been developed that involve a mixture of wave and ray dynamics. They have been shown to be highly efficient on realistic electromagnetic applications involving homogeneous and inhomogeneous media for various irregular exterior domains geometries.

- *Meteorology*

  In collaboration with J.R. Bates and Yong Li of NASA/Goddard, we developed a multilevel semi-implicit, semi-Lagrangian method for shallow water equations, based on potential vorticity and divergence, that has proved to be more efficient and much more flexible than methods currently used in numerical weather prediction. In collaboration with Sam Yee of the Phillips Laboratory at Hanscomb AFB, we have developed effective multilevel local refinement techniques for this approach.

- *Multiscale Atmospheric Data Assimilation*

  The main bottleneck today in atmospheric and oceanic flow calculations is the need to assimilate into them a continuously incoming, extremely non-uniform stream of measurement data: optimal assimilation requires the solution of a huge n by n dense system of equation. Investigating the problem over the last year, we have found that multiscale methods can solve such problems in just O(n) operations. Multiscale data assimilation may in fact be even faster than direct flow simulation itself.

- *Molecular Dynamics*

  The cost of simulating macromolecular dynamics by current state-of-the-art methods rises very steeply with problem size. Our studies, including numerical

tests on simplified models, have shown that this steep rise in cost can be radically reduced by multiscale algorithms.

- *Robust Three-Dimensional Solvers*

  In collaboration with Uri Shumlak of the Phillips Laboratory at Kirtland AFB, we have developed a very efficient and robust three-dimensional multigrid solver that is well-suited to parallel computation.

- *Parallel Adaptive Refinement*

  Work has continued on the development of AFACx for more general applications (AFACx is a multilevel refinement method that allows for effective simultaneous computation on all levels) and AMR++ for a broad range of machines and capabilities (AMR++ is a C++ software development environment that supports general code production but provides automatic and efficient application to a host of advanced computers).

Before the mid 1980s, multilevel methods were slow to find their way into applications codes. While not unusual for new advances, the pace for multilevel methods seemed slower than one might expect. One of the likely causes was the beginning misconceptions about multilevel capabilities, fed by frequent failures of early developments. However, the situation today is drastically different. By the late 1980s, multigrid methods were already becoming commonplace in codes of certain application areas and they were rapidly appearing in others. For recent development, see the information and codes accessible through MGNet, especially papers from the Sixth and Seventh Copper Mountain Conferences on Multigrid Methods: ftp://na.cs.yale.edu/pub/mgnet/www/mgnet or http://na.cs.yale.edu/mgnet/www/mgnet.html. It is worth noting that the computational approaches developed over the past several years in our research on high-performance CFD (introducing advanced nonelliptic multigrid methods) are in the core of a major project now being proposed by several senior investigators (headed by Dr. Jerry South) at NASA/Langley. Their purpose is to develop, by year 2000, multigrid solvers for 3-D aerodynamics that will be two orders of magnitude faster than current solvers.

An important ingredient in the effective progress of an evolving discipline is the organized dissemination of developing knowledge. The project team has been actively involved in such technology transfer, starting with the Multigrid Workshop at ICASE in 1978. To date in the U.S. alone, the proposers have organized seven Copper Mountain conferences, three major workshops, four short courses, and eight tutorials. In addition, the proposers have developed texts, guidebooks, bibliographies, videotaped lectures, and curriculum, and have acted as a resource of information and informal consultation.

There are many aspects of the current research project that have influenced—and have been influenced by—the work of others through collaboration and informal discussion. For example, there continue to be many short term visitors, institutional

affiliates, and informal collaborating scientists who have interacted with research and development aspects of the project. Moreover, there were two post doctorates and two sabbatical visitors who worked directly on project activities. While such support was not a formal part of the AFOSR funded project, this mutual interaction with collaborators was essential to its relevance and progress.

Further Information

More information on these topics (including algorithm details, theoretical and numerical results, practical applications, and historical and philosophical perspectives) can be obtained via anonymous ftp at

amath.colorado.edu/pub/multigrid

and

amath.colorado.edu/pub/fosls

or via the World Wide Web at

http://amath-www.colorado.edu/appm/faculty/stevem/Home.html.

References

[1] Balsara, D. and Lemke, M. and Quinlan, D., AMR++, a C++ Object Oriented Class Library for Parallel Adaptive Refinement Fluid Dynamics Applications, in *Proceedings of American Society of Mechanical Engineers,* vol. 157, pp. 413–433, AMD, 1992.

[2] Bates, J.R., Y. Li, A. Brandt, S. F. McCormick and J. Ruge, A global shallow water numerical model based on the semi-Lagrangian advection of potential vorticity, *Quart. J. Roy. Met. Soc.,* in press.

[3] Bochev, P. Z. Cai, T. Manteuffel, and S. McCormick, First-order system least squares for the velocity-pressure-velocity-flux form of the Navier-Stokes equations, in progress.

[4] Brandt, A., Multiscale computational methods: research activities. In: *Proc. 1991 Hang Zhou International Conf. on Scientific Computation* (T. Chan and Z.-C. Shi, eds.), World Scientific Publishing Co., Singapore, 1992, pp. 1–7.

[5] Brandt, A. and C.H. Venner, Multilevel evaluation of integral transforms with asymptotically smooth kernels. Gauss Center Report WI/GC–2, The Weizmann Inst. of Science, April 1995.

[6] Brandt, A. and L.Y. Zaslavsky, Multilevel algorithm for atmospheric data assimilation. Part I. Multiscale iterative process. *Proc. CCMM95* (1995).

[7] Cai, Z., R. D. Lazarov, T. Manteuffel, and S. McCormick, First-order system least squares for second-order partial differential equations: Part I, *SIAM J. Numer. Anal.,* **31** (1994), pp. 1785-1802.

[8] Cai, Z., T. Manteuffel, and S. McCormick, First-order system least squares for second-order partial differential equations: Part II, *SIAM J. Numer. Anal.,* to appear.

[9] Cai, Z., T. Manteuffel and S. McCormick, First-order system least squares for the Stokes equations , with application to linear elasticity, *SIAM J. Numer. Anal.,* to appear.

[10] Cai, Z., T. Manteuffel, S. McCormick and S. Parter, First-order system least squares for elasticity, submitted.

[11] Lemke, M and D. Quinlan, P++, a C++ virtual shared grids based programming environment for architecture–independent development of structured grid applications, in *Lecture Notes in Computer Science,* vol. 634, Springer–Verlag, Berlin, 1992.

[12] Lemke, M., K. Witsch and D. Quinlan, An object–oriented approach for parallel self adaptive mesh refinement on block structured grids, in *Sixth Copper Mountain Conference on Multigrid Methods,* vol. CP3224, pp 345–359, N. D. Melson and T. A. Manteuffel and S. F. McCormick, eds., NASA, Hampton, VA, 1993.

[13] Livshits, Irina, Ph.D. thesis, in preparation.

[14] Manteuffel, T. and S. McCormick, Multilevel projection methods for first-order system least squares, *Procs. ASME Fluids Eng. Div. Summer Mtg.,* Lake Tahoe, CA, June 9-23, 1994.

[15] Manteuffel, T., S. McCormick, and G. Starke, First-order system least squares for elliptic problems with discontinuous coefficients, manuscript.

[16] McCormick, S., *Multilevel Projection Methods for Partial Differential Equations*, CBMS–NSF, vol. 62, SIAM Books, Philadelphia, 1992.

[17] McCormick, S., Multilevel projection methodology, *Procs. CTAC Conference,* Austr. Natl Univer., May, 1993.

[18] McCormick, S., Multilevel first-order system least-squares (FOSLS) for Helmholtz equations, *Procs. 2nd Intl Conf. on Approx. and Num. Meths. for the Solution of the Maxwell Equations,* Wash. D.C., John Wiley and Sons, Oct., 1993.

[19] Ruge, J.W., Y. Li, S.F. McCormick, A. Brandt and J.R. Bates, A nonlinear multigrid solver for a semi-Lagrangian potential vorticity based shallow water model on the sphere, *SIAM J. Sci. Comput.,* submitted.

[20] Ruge, J.W., S.F. McCormick and S. Yee, Multilevel adaptive methods for semi-implicit solution of shallow water equations on the sphere, *Mon. Wea. Rev.,* **123** (1995), 2197-2205.

[21] Schaffer, S., A semi-coarsening multigrid method for elliptic partial differential equations with highly discontinuous and anisotropic coefficients, *SIAM J. Sci. Stat. Comp.,* submitted.